SUPERCOMPUTING

AND

THE HUMAN ENDEAVOR

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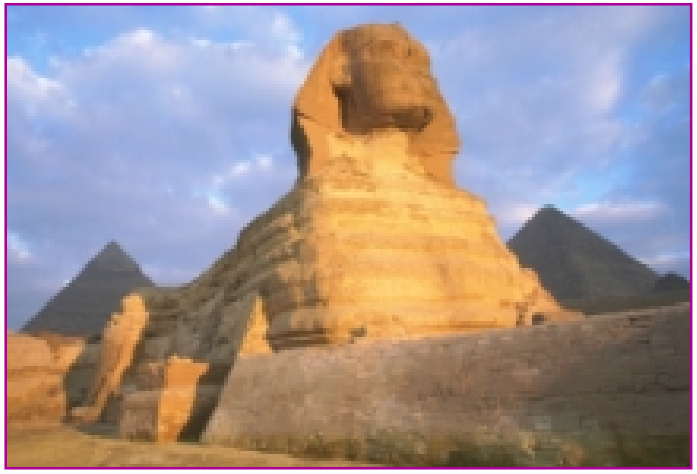
The world is on the verge of three great revolutions

- **A revolution in biology**
  - *Especially in the exploitation of the human genome*
- **A revolution in supercomputing**
  - *Changing the way that we use machines to help us think*
- **A social revolution in how we come to grips with the first two revolutions**

Galileo

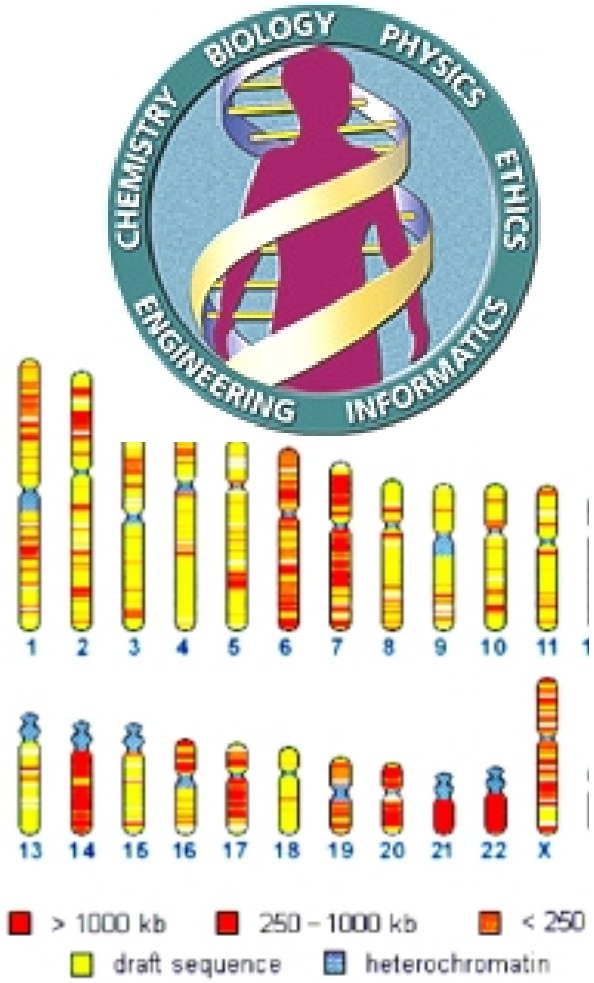
To first order, human beings today are the same as at the beginning of recorded history

- **The historical record stretches only 5 millennia**
- **Insufficient time for any appreciable change in the human genome**
- **Physically we are the same**
  - *A little taller (protein)*
  - *Live longer (medicine)*
- **We face the same problems**
  - *Raising a family*
  - *Running an equitable society*
  - *Distrust of other cultures*
  - *Quest for understanding of the universe and our place in it*



The revolution in the biological sciences is the first opportunity to make significant changes to the human body

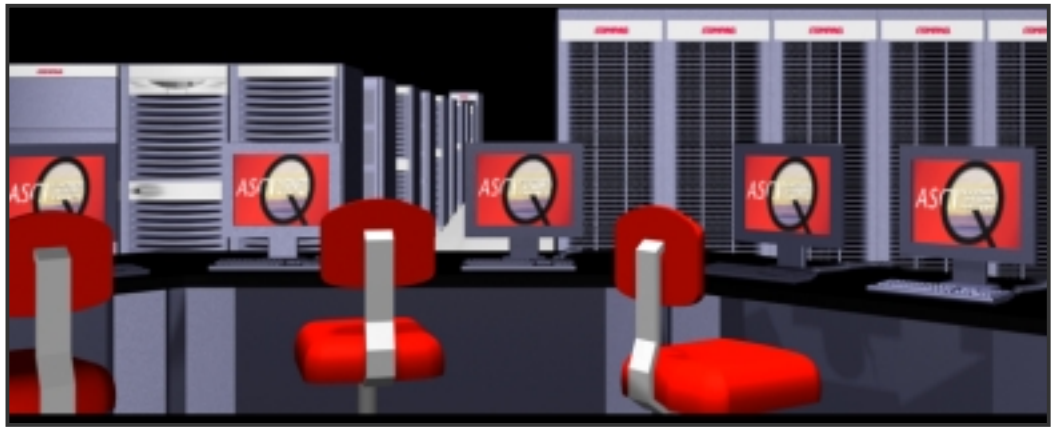
- **Eliminate genetic diseases**
- **Prolong life**
- **"Improve" physical and mental capabilities**
- **But - there are significant ethical and social issues**
  - *Will these discoveries be used to "engineer" human beings?*
  - *Will unique aspects of humanity, including diversity, be lost on the altar of "better"?*



The revolution in supercomputing has simultaneous opportunities and challenges

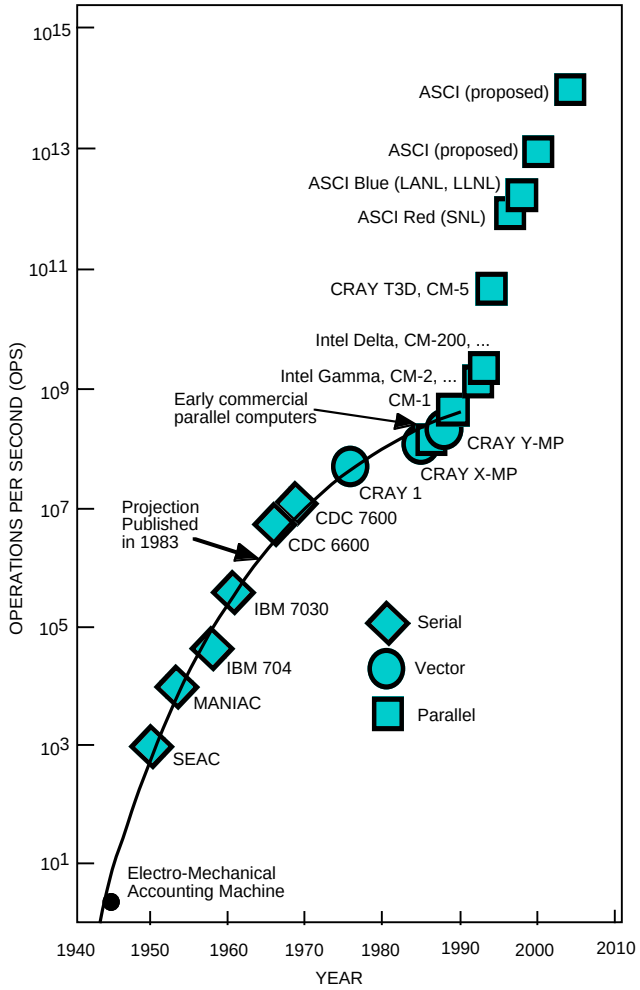
- **Until now computers have been mainly:**
  - *Fast calculators*
  - *Simulators of reality*
- **Until now we have interacted with the computer on the computer's terms**
- **Until now there have been relatively few ethical or social issues associated with computing**

This is about to change



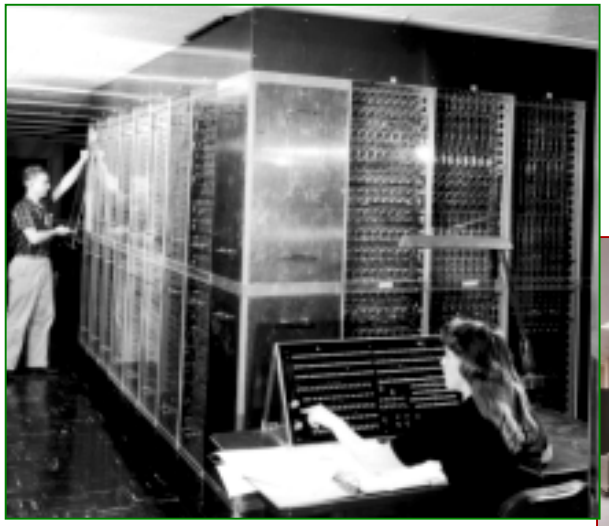
The technological progress in supercomputing is one of the greatest technical achievements of humankind

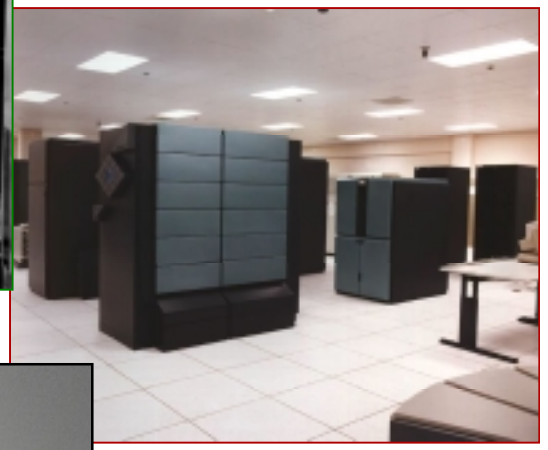
- 1940's: "Computers" were human beings with adding machines
- 1950's: Computers were huge machines with vacuum tubes and relays - few users
- 1960's: Science and business began use of electronic computers
- 1970's: Personal computers
- 1980's: The last single processor supercomputers
- 1990's: Parallel supercomputers
- 2000's: Networked supercomputers of revolutionary capability

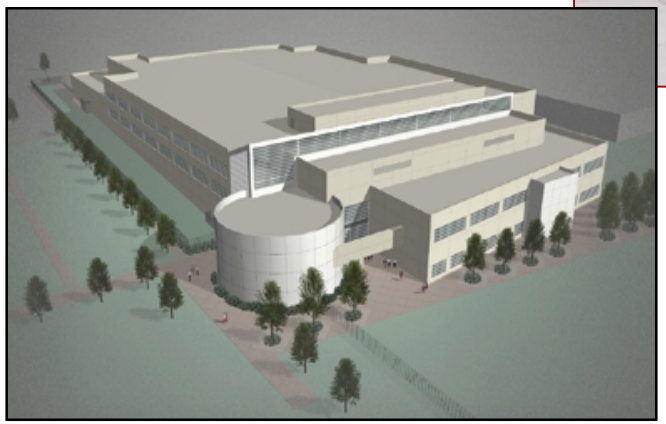


Los Alamos has played a key role in the development of supercomputing

- Manhattan Project: Our "computer" was a room full of women with mechanical calculators
- Los Alamos built one of the first electronic computers
- Los Alamos had the first Cray computer (serial number 1)
- Los Alamos exploited massively parallel supercomputers
- The Strategic Computing Complex will house "Q" - the world's most powerful supercomputer (30 TeraOps)







DOE's Accelerated Strategic Computing Initiative (ASCI) is driving supercomputer technology

- **Key to maintaining the nuclear weapons stockpile without testing**
- **Uses commercially available hardware linked together to make unique computational resources**
- **ASCI consists of four major elements:**
  - *Hardware*
  - *Applications software*
  - *Environment*
  - *Verification and validation*
- **ASCI is a partnership of government, laboratories, universities, and industry**

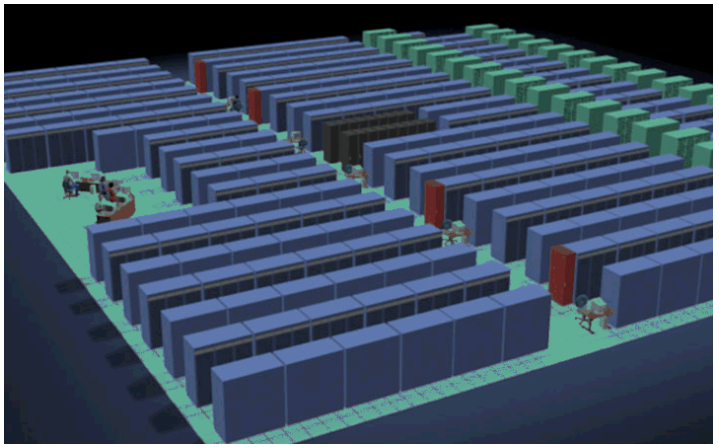

Blue Pacific


Blue Mountain


ASCI Red

Within the decade we will have machines capable of Peta-Op speeds (10^{15} operations/sec)

- **More than just bigger and faster**
- **Will open up whole new classes of investigation**
- **Will enable us to interact with computers on a human level**
  - *Plain language*
  - *"Intelligent" responses*



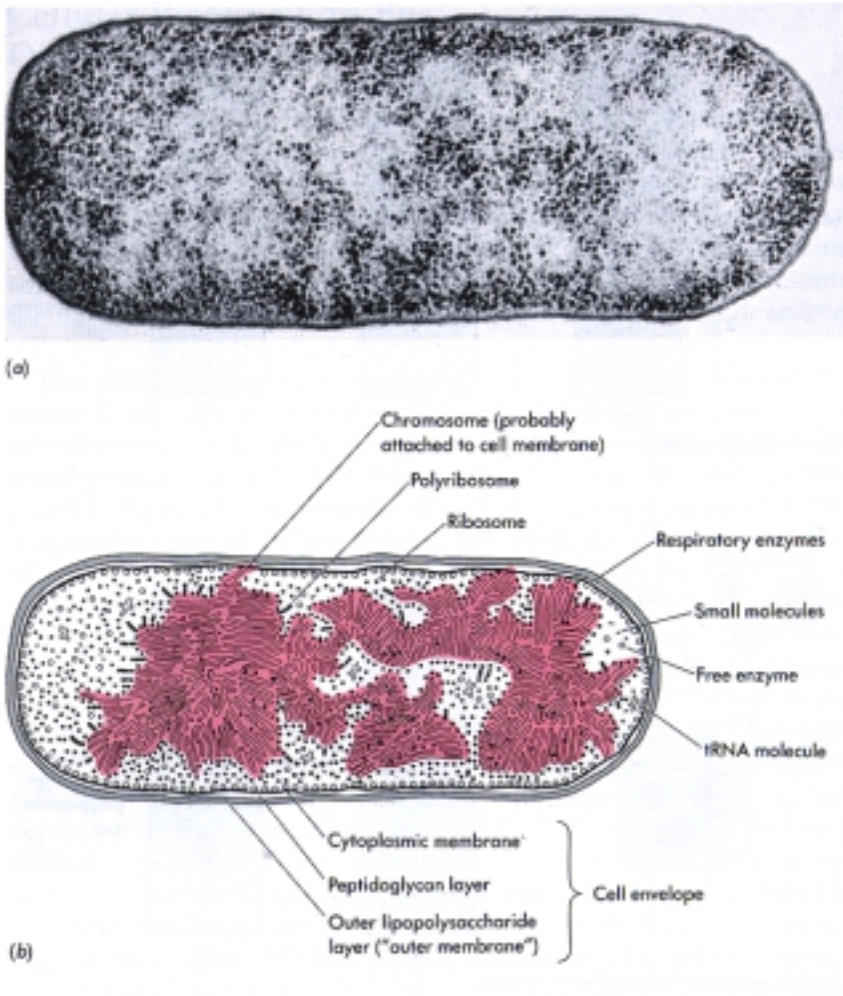
More than a "grand challenge" - this is a true scientific revolution

What would you do with a computational engine of *unlimited capability*?

- **More than "what we are doing now, only bigger and faster"**
- **What are the great intellectual questions that we might use these machines to help us answer?**
  - *Understanding the processes of life*
  - *Understanding processes of the brain*
  - *Simulation of extraordinarily complex phenomena*
- **Other applications**
  - *Driving the future knowledge economy*
  - *Making sense of the information explosion*

At one PetaOp one can begin to think about simulating a living object, atom-by-atom

- **E. coli bacterium**
  - *Molecular weight: 10^{12}*
  - *Length: 2 microns*
  - *Diameter: 1 micron*
  - *70% water*
  - *10^6 protein molecules*
  - *3000-6000 different types of molecules*
  - *Reproduces every 20 minutes in an appropriate medium*



Rough estimate of computer requirements for atom-by-atom simulation of E. coli

- **Molecular dynamics simulation of E. coli bacterium**
- **10^{11} atoms in bacterium**
- **Ten times that number of atoms in surrounding media**
  - *Total atoms in simulation: 10^{12} atoms*
- **Memory required: Few tens of terabytes**
- **Assume that of order 100 operations required per atom per timestep**
  - *This implies 10^{14} operations per molecular dynamics timestep*
- **Approximate time required on various computers for one timestep:**
  - *Blue Mountain (3 TeraOps): 33 seconds*
  - *Q (30 TeraOps): 3.3 seconds*
  - *One PetaOp Computer (2006?): 0.1 second*

The principal challenge for the E. coli simulation is computer speed

- **Memory is no problem - "only" tens of terabytes**
- **On a 1 PetaOp computer:**
  - *0.1 second per timestep*
  - *Timestep determined by velocity of atoms, distance between*
  - *For 1 Angstrom and room temperature: $dt=4x10^{-15}$ seconds*
  - *With thermal averaging, might get increase of 1000*
  - *Net timestep could be as high as 10^{-12} seconds*
  - *One year of computer time: 0.0003 seconds simulation time*
    - Millionths of a bacterial generation
    - A start, but still not there without algorithmic development

Computational difficulties are not the only challenge in simulating a living object

- **Must know detailed chemical structure to begin simulation**
- **Must have adequate force fields for simulation**
- **However - *"even a cautious chemist, when properly informed, need not look at a bacterial cell as a hopelessly complex object. Instead he might easily adopt an almost joyous enthusiasm, for it is clear that he…at last possesses the tools to describe completely the essential features of life"***
  - *James Watson, "Molecular Biology of the Gene," Second Edition, 1970*

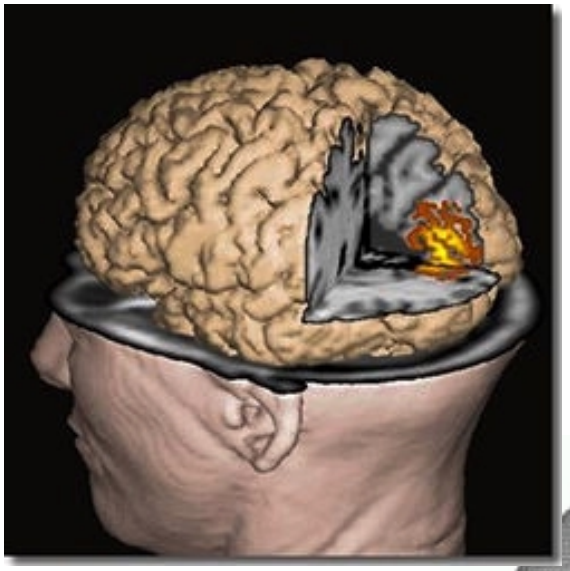
Simulating the processes of life is much more than a scientific tour de force

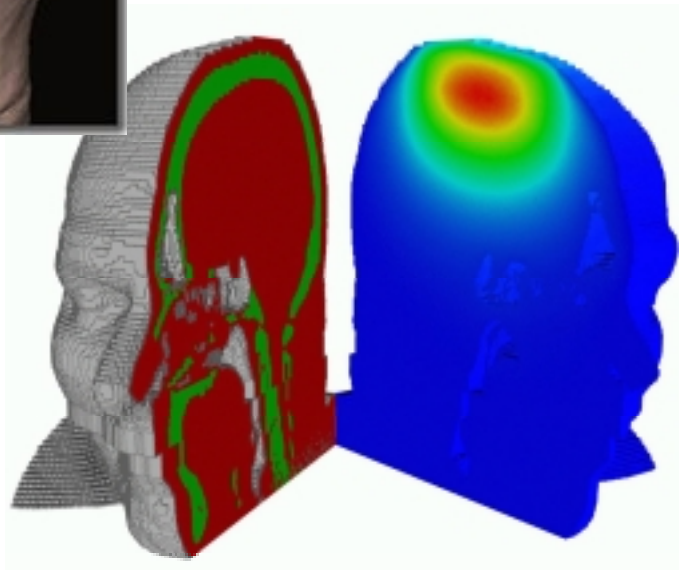
- **Touches upon questions that have been asked for as long as human beings have asked questions**
  - *What is life?*
  - *What is the difference between living matter and dead matter?*

- **What are the other applications of this technology?**
  - *Understanding diseases and their cures*
  - *Understanding aging and how it might be controlled*

At one PetaOp one can begin to think about modeling a complex animal brain

- Human cerebral cortex contains ~10^{12} neurons
- Octopus performs complex motor tasks with $5x10^{6}$ neurons
- Bumble bees can fly and work with only 100,000 nerve cells
- C. elegans worm has only 300 neurons
- Simulations can model each neuron and synapse
  - *Sensory input*
  - *Motor output*





What can modeling the brain tell us about what it means to be human?

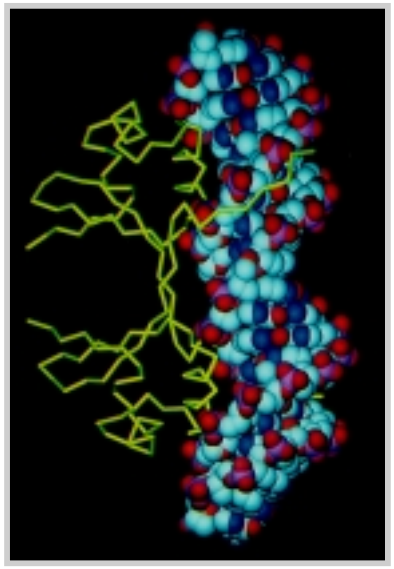
- **A better understanding of how we perceive the world**
- **May allow the quantitative study of some forms of mental illness**
  - *Is mental illness purely chemical or structural?*
  - *How do complex "experiences" affect mental development?*
- **What would other, non-human, forms of "intelligence" be like?**

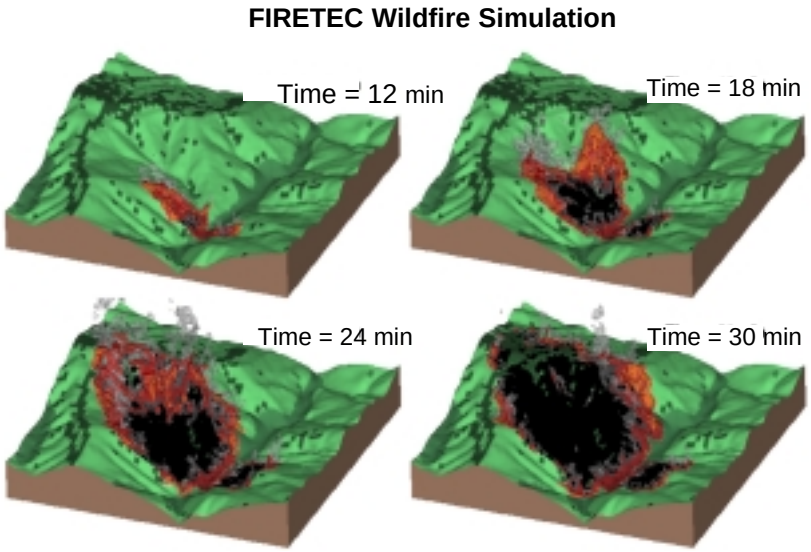
These examples are more than just “grand challenges” - they are “meta-problems”

- **Topics that until recently were the domain of the humanist**
  - *Psychology and psychiatry*
  - *Theories of life*
  - *Knowledge and learning*
- **Supercomputers represent a new way of looking at ourselves and the world**
  - *As profound as the introduction of experimentation by Bacon and Galileo*
  - *As profound as the industrial revolution’s spread of technology*

Practical applications: Supercomputers will enable simulations of extraordinary complexity

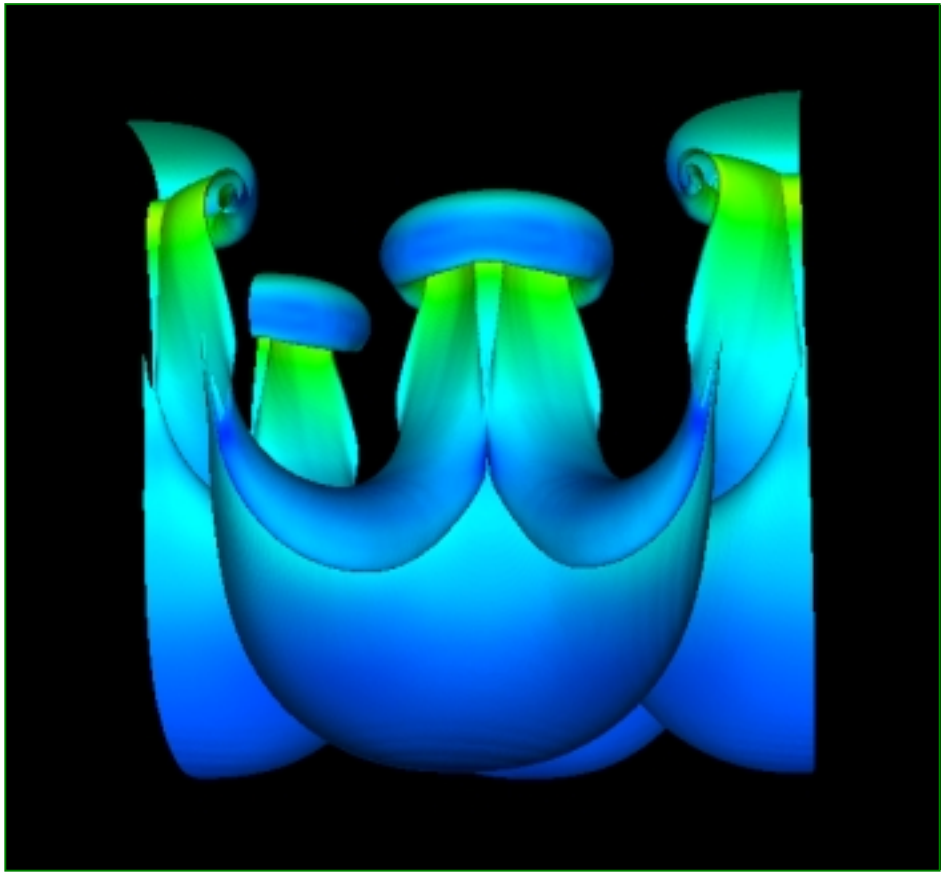
- **Chemistry**
  - *Designer materials*
- **Molecular biology**
  - *Protein folding*
- **Engineering design**
  - *Microchips to motorcycles*
- **Weather and oceans**
  - *Global warming*
- **Forest fires**
  - *Couple weather into predictions*
- **Social modeling**
  - *Traffic, trends, sociology, environment*
- **Education, training, entertainment**
  - *Reading, flying, fun*





Supercomputing is the keystone for the success of stockpile stewardship

- **Without nuclear testing, large-scale simulation is the only way to assure the safety and performance of weapons**
- **Blue Mountain has already enabled simulations that would have taken *centuries* on previous machines**
- **Estimates are that a 100 TeraOp machine is required for a reasonable simulation of a complex nuclear device**
- **DOE's ASCI program is driving supercomputing technology**



Supercomputers will challenge our most cherished methods of theoretical physics

- **Many current computational techniques date from the 1930's or even earlier**
  - *Partial differential equations*
  - *Numerical solutions on a mesh*
- **What new techniques might be used to exploit the unique features of massively parallel computers?**
  - *Brute force solution of equations?*
  - *Cellular automata-like methods?*
  - *Statistical approaches?*
- **This is a rich field for creative research**
  - *Requires a blend of physics, computational methods, computer science*

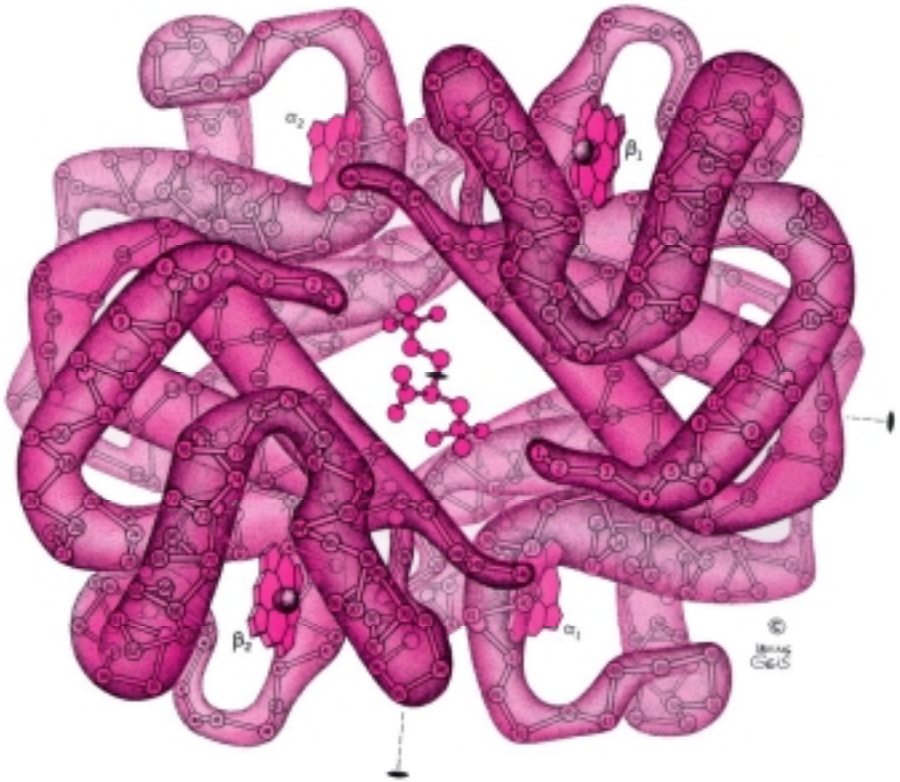
“Concurrent simulation” would link supercomputers with experiments in real time

- **Traditionally computers have been used to**
  - *Control experiments*
  - *Record data*
  - *Analyze data*

- **Fast large computers could perform simulations while the experiment is in progress**
  - *Not just “calculate and compare after the experiment”*
  - *Simulations “learn from” the experiment and make adjustments in real time*

Supercomputers are already beginning to link physics and biology

- **The two scientific revolutions are linked**
- **Utilization of the decoding of the human genome**
  - *What are the causes of disease?*
  - *How might we prevent / treat them?*
- **Rational drug design will enable the design of drugs tuned to the individual**
  - *Free of side effects*
  - *Chemotherapy from art to science*



Complex Protein Molecule

Supercomputers will be drivers of the future "knowledge economy"

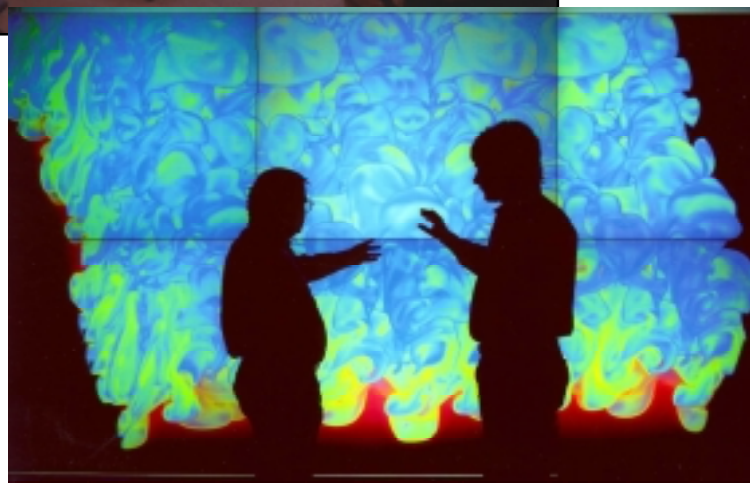
- Innovation will be the economic driver of the future
- Time to market is the key to profitability
- Supercomputers will allow better simulation and hence save on prototyping
- Countries with advanced capabilities in computing will dominate the high technology industries of the future

Supercomputers will enable “new ways of using machines to help us think”

- The information explosion is breathtaking
- How to find what you’re looking for?
- How to find it in a format that you can use?
- Supercomputers will enable the internet to serve its true purpose - to promote knowledge, understanding and interactions in human beings

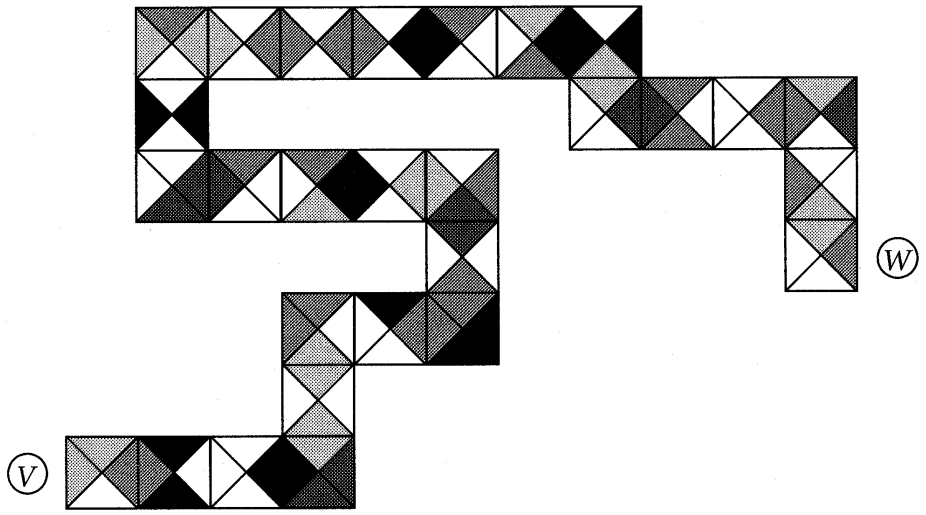
How we interact with computers will change profoundly over the next decade

- **Until now we have interacted with computers on their terms:**
  - *Keyboard, mouse, touchscreen, projected display, ...*
- **In the future computers will be fast enough to speak with us and even understand what we wish to learn and understand**



What can't supercomputers do? Understanding the limits of computation

- **We already know that long-range weather predication is impossible**
  - *After about 30 days the atmosphere becomes chaotic*
- **Some classes of problems in logic, number theory, and geometry are known to be unsolvable on computers of any speed and size**
- **Unanswered question: Can a computer be "intelligent"?**

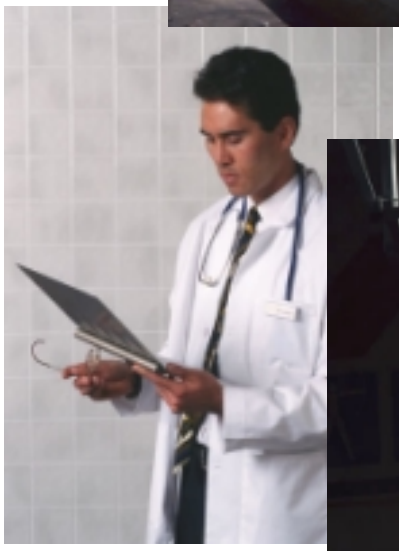


A domino snake connecting *V* to *W*

It is impossible to produce a computer “duplicate” of an individual human mind

- The human brain is chemical
- Chemistry is governed by quantum mechanics
- Uncertainty subtly affects molecular reactions in the brain
- Any two identical “brains” will diverge with time
- And: The “mind” is more than the physical structure and function of the brain



The third revolution: Significant ethical and social issues associated with the scientific revolutions in biology and supercomputing

- **Will understanding how the human brain works make us "less human"?**
  - *Will such knowledge be used for psychological warfare?*
- **What are the religious implications of understanding the detailed processes of life?**
  - *If we understand the body completely, what is the soul?*
- **What are the philosophical issues associated with simulations that have a "reality" of their own?**
  - *More than just a video game!*
- **What are the economic social, and political implications of a quantum leap in the "digital divide" between rich and poor?**

Every revolution brings unique ethical challenges and choices

- **Political revolutions**
  - *Violent social change*
- **Industrial revolutions**
  - *Pollution, economic change*
- **Scientific revolutions**
  - *Change in world view*
- **History can be viewed as a sequence of increasingly complex choices**
- **It is within our power to make the revolution in supercomputing an opportunity and not a threat**

"Supercomputing and the Human Endeavor"
A conference to be held in June, 2001

- **Collaboration between:**
  - *Los Alamos National Laboratory*
  - *Woodrow Wilson Center for Scholars (Washington, DC)*
- **Bring together a diverse set of thinkers:**
  - *Computer scientists and engineers*
  - *Physical and biological scientists*
  - *Historians*
  - *Ethicists*
  - *Government leaders*
- **What are the social and ethical implications associated with the coming scientific revolution in supercomputing?**

Los Alamos is taking a leading role in the revolution in supercomputing

- **Big machines**
  - *Blue Mountain*
  - *Q*
- **Big codes**
  - *Unprecedented simulations*
- **New forms of visualization**
- **New frontiers in computer science**
- **Conference on social and ethical implications (6/01)**
- **“Out of the box” thinking welcome here!**
  - *What are the great problems that we can help solve?*